



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:57 PM EDT

PDB ID : 1FCJ
Title : CRYSTAL STRUCTURE OF OASS COMPLEXED WITH CHLORIDE AND SULFATE
Authors : Burkhard, P.; Tai, C.; Jansonius, J.N.; Cook, P.F.
Deposited on : 2000-07-18
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

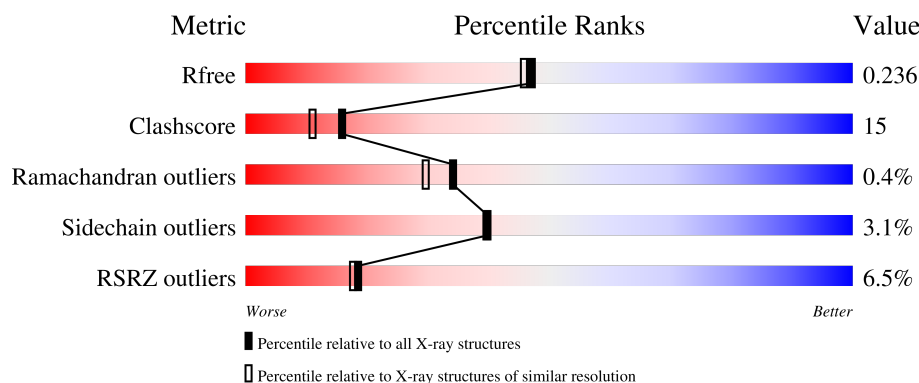
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	<div> <div>3%</div> <div>73%</div> <div>19%</div> <div>6%</div> </div>
1	B	322	<div> <div>7%</div> <div>70%</div> <div>22%</div> <div>6%</div> </div>
1	C	322	<div> <div>12%</div> <div>70%</div> <div>23%</div> <div>6%</div> </div>
1	D	322	<div> <div>3%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called O-ACETYLSELINE SULFHYDRYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2251	1418	390	437	6			
1	B	304	Total	C	N	O	S	0	0	0
			2271	1429	395	441	6			
1	C	304	Total	C	N	O	S	0	0	0
			2271	1429	395	441	6			
1	D	302	Total	C	N	O	S	0	0	0
			2251	1418	390	437	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	VAL	CONFLICT	UNP P0A1E3
A	267	ILE	PHE	CONFLICT	UNP P0A1E3
B	266	GLY	VAL	CONFLICT	UNP P0A1E3
B	267	ILE	PHE	CONFLICT	UNP P0A1E3
C	266	GLY	VAL	CONFLICT	UNP P0A1E3
C	267	ILE	PHE	CONFLICT	UNP P0A1E3
D	266	GLY	VAL	CONFLICT	UNP P0A1E3
D	267	ILE	PHE	CONFLICT	UNP P0A1E3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

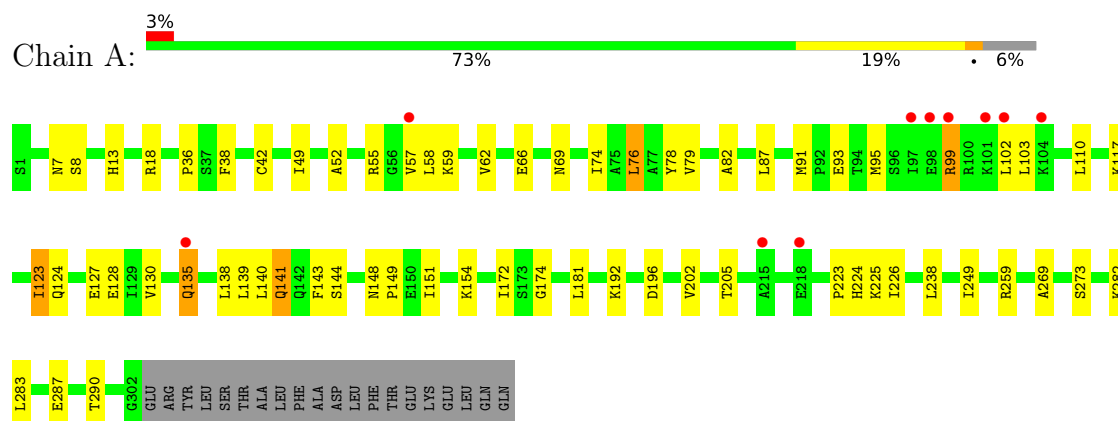
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	286	Total	O	0	0
			286	286		
5	C	260	Total	O	0	0
			260	260		
5	D	290	Total	O	0	0
			290	290		

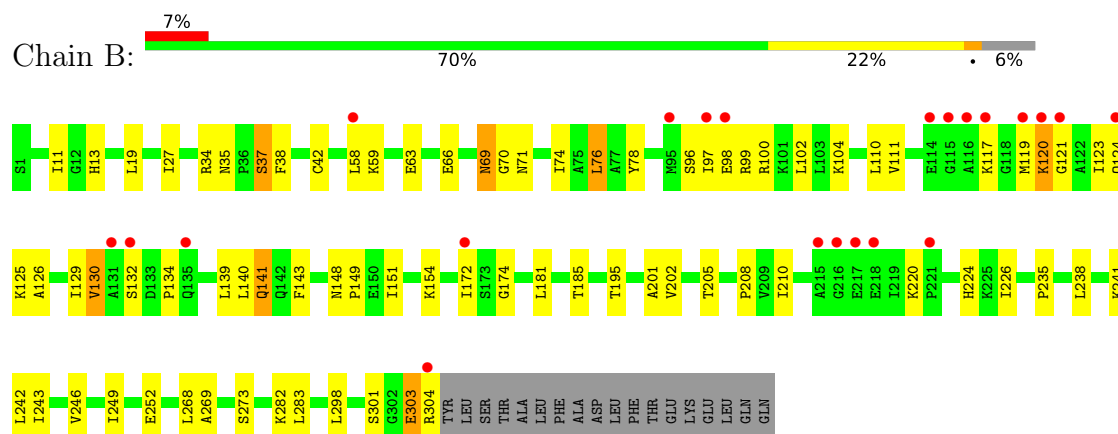
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

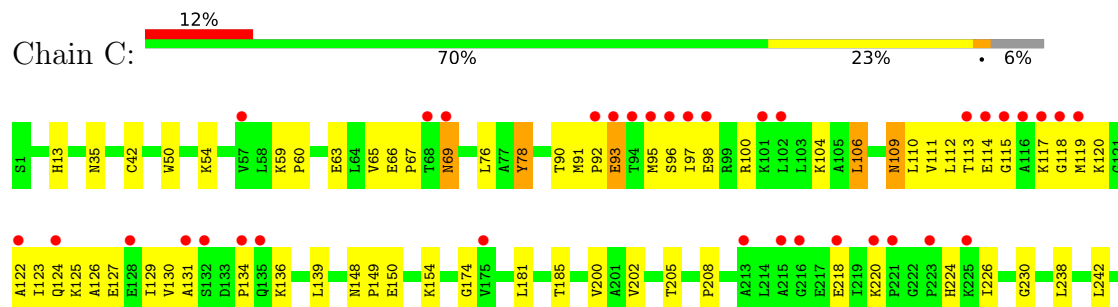
• Molecule 1: O-ACETYLSELINE SULFHYDRYLASE

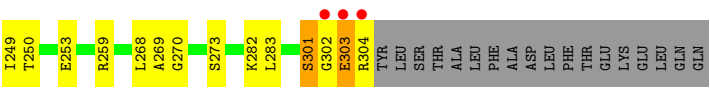


• Molecule 1: O-ACETYLSELINE SULFHYDRYLASE

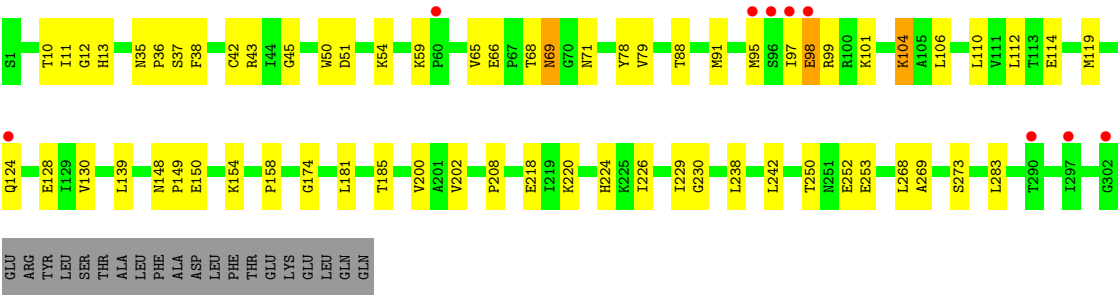
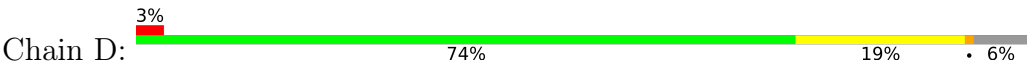


• Molecule 1: O-ACETYLSELINE SULFHYDRYLASE





● Molecule 1: O-ACETYLSERINE SULFHYDRYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 100.49Å 142.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.13 – 2.00 28.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.7 (28.13-2.00) 89.4 (28.13-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.246 0.193 , 0.236	Depositor DCC
R_{free} test set	4530 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10246	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7990e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PLP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/2282	0.76	1/3089 (0.0%)
1	B	0.51	0/2302	0.75	1/3115 (0.0%)
1	C	0.50	0/2302	0.75	1/3115 (0.0%)
1	D	0.55	0/2282	0.75	0/3089
All	All	0.52	0/9168	0.75	3/12408 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	GLU	N-CA-C	-7.29	91.32	111.00
1	A	18	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	298	LEU	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2251	0	2331	71	0
1	B	2271	0	2350	74	0
1	C	2271	0	2350	68	0
1	D	2251	0	2331	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	7	0	0
4	B	15	0	6	1	0
4	C	15	0	7	0	0
4	D	15	0	7	1	0
5	A	282	0	0	21	0
5	B	286	0	0	28	0
5	C	260	0	0	16	0
5	D	290	0	0	24	0
All	All	10246	0	9389	270	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 270 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:HE3	1:B:120:LYS:H	1.16	1.08
1:A:290:THR:HB	5:A:3148:HOH:O	1.56	1.04
1:C:65:VAL:HB	5:C:3156:HOH:O	1.59	1.02
1:A:42:CYS:HB3	5:A:3115:HOH:O	1.61	0.99
1:D:43:ARG:HG2	5:D:3293:HOH:O	1.68	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/322 (93%)	292 (97%)	8 (3%)	0	100	100
1	B	302/322 (94%)	289 (96%)	11 (4%)	2 (1%)	22	16
1	C	302/322 (94%)	287 (95%)	12 (4%)	3 (1%)	15	9
1	D	300/322 (93%)	291 (97%)	9 (3%)	0	100	100
All	All	1204/1288 (94%)	1159 (96%)	40 (3%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	303	GLU
1	B	132	SER
1	C	69	ASN
1	B	141	GLN
1	C	93	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/259 (93%)	234 (97%)	7 (3%)	42	43
1	B	243/259 (94%)	234 (96%)	9 (4%)	34	32
1	C	243/259 (94%)	237 (98%)	6 (2%)	47	49
1	D	241/259 (93%)	233 (97%)	8 (3%)	38	37
All	All	968/1036 (93%)	938 (97%)	30 (3%)	40	40

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	LEU
1	D	158	PRO
1	C	106	LEU

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Mol	Chain	Res	Type
1	D	238	LEU
1	D	78	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	135	GLN
1	D	69	ASN
1	C	13	HIS
1	D	13	HIS
1	B	224	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	2003	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	A	2001	-	4,4,4	0.15	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLP	C	3002	1	15,15,16	1.13	1 (6%)	20,22,23	1.09	2 (10%)
4	PLP	D	3004	1	15,15,16	1.39	2 (13%)	20,22,23	1.07	2 (10%)
4	PLP	B	3003	1	15,15,16	1.38	1 (6%)	20,22,23	1.21	2 (10%)
4	PLP	A	3001	1	15,15,16	1.11	1 (6%)	20,22,23	1.09	2 (10%)
2	SO4	C	2002	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	D	2004	-	4,4,4	0.28	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	C	3002	1	-	1/6/6/8	0/1/1/1
4	PLP	D	3004	1	-	0/6/6/8	0/1/1/1
4	PLP	B	3003	1	-	0/6/6/8	0/1/1/1
4	PLP	A	3001	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3004	PLP	C3-C2	-3.57	1.37	1.40
4	B	3003	PLP	C3-C2	-3.35	1.37	1.40
4	C	3002	PLP	C3-C2	-2.48	1.38	1.40
4	A	3001	PLP	C3-C2	-2.31	1.38	1.40
4	D	3004	PLP	C5-C4	-2.19	1.38	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3003	PLP	O4P-C5A-C5	2.66	114.42	109.35
4	C	3002	PLP	O4P-C5A-C5	2.43	113.99	109.35
4	D	3004	PLP	O3P-P-O1P	2.32	119.77	110.68
4	A	3001	PLP	O3P-P-O1P	2.29	119.66	110.68
4	D	3004	PLP	O4P-C5A-C5	2.23	113.60	109.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3002	PLP	C5A-O4P-P-O1P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3004	PLP	1	0
4	B	3003	PLP	1	0
2	D	2004	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/322 (93%)	0.22	10 (3%) 46 45	13, 23, 43, 56	0
1	B	304/322 (94%)	0.37	22 (7%) 15 14	14, 25, 54, 73	0
1	C	304/322 (94%)	0.57	38 (12%) 3 3	14, 26, 62, 76	0
1	D	302/322 (93%)	0.16	9 (2%) 50 49	13, 22, 40, 53	0
All	All	1212/1288 (94%)	0.33	79 (6%) 18 18	13, 24, 52, 76	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	ALA	5.8
1	C	97	ILE	5.8
1	C	216	GLY	5.6
1	C	95	MET	5.5
1	B	116	ALA	5.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	2002	5/5	0.94	0.12	46,52,57,59	0
2	SO4	D	2004	5/5	0.95	0.13	44,45,46,54	0
2	SO4	B	2003	5/5	0.98	0.08	37,38,44,44	0
3	CL	D	2008	1/1	0.98	0.14	37,37,37,37	0
4	PLP	A	3001	15/16	0.98	0.14	10,16,19,20	0
4	PLP	B	3003	15/16	0.98	0.13	15,20,25,26	0
4	PLP	C	3002	15/16	0.98	0.15	18,21,26,27	0
2	SO4	A	2001	5/5	0.99	0.11	22,28,35,36	0
3	CL	A	2006	1/1	0.99	0.12	24,24,24,24	0
3	CL	B	2007	1/1	0.99	0.13	28,28,28,28	0
3	CL	C	2005	1/1	0.99	0.10	23,23,23,23	0
4	PLP	D	3004	15/16	0.99	0.16	12,17,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.